CHBE 611
Graduate Thermodynamics

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Spring 2021

Office: B235 Abercrombie	Office Hours: TBD
Class Room: DCH 1046	Class Hours: 8 AM - 9:15 AM T, Tr HRZ Amp
Recitation	Hours: Friday (time TBD)

Teaching assistant

TBD

Navigating around Covid

Following the university guidelines, till middle of February we will hold the class online. Once the university allows in-person instruction, we will switch to the in-person format. We will also plan to broadcast the lectures, so students who stay home can still take the classes. The course description and approach laid out below will mostly hold even factoring Covid-induced limitations. However, if need be, we will make changes to the syllabus to deal with any potential issues due to the continuing pandemic.

Course Description

Thermodynamics deals with the restriction and interrelation amongst the properties that we use to characterize matter. A distinguishing feature of thermodynamics is its generality in applying to all types of systems in macroscopic aggregation. Statistical mechanics, on the other hand, provides a framework to infer the macroscopic properties of a system from the underlying microscopic physics. The *inferential perspective* of thermodynamics is most clearly seen from the statistical point of view. The inferential development traces back to Gibbs and the information theoretic development by Jaynes; this is the perspective that we will develop in this course. Our plan is to develop the concepts from the microscopic perspective and study simple, yet realistic problems that one encounters in chemical and bio-molecular sciences. From this vantage, we will seek a renewed appreciation of classic thermodynamics, including of mixtures and solutions.

Topics to be covered

The “chapters" noted below are from my course notes.

1. Overview of thermodynamics and statistical mechanics
2. Review (*self-study using Chapter1.pdf*)
    - Characterizing thermodynamic systems, controllable variables & measurability, energy conservation, and the nature of heat
    - Driving forces and conditions of equilibrium
    - Euler’s relation and the Gibbs-Duhem equation
    - Fundamental equation of state, alternative representations, and thermodynamic potentials
3. Review of mechanics, symmetries and conservation (*Chapter3.pdf*)
4. Liouville’s theorem and its consequences (*Chapter4.pdf*)
5. Microcanonical and Canonical Ensembles from Gibbs’ perspective (*Chapter5.pdf*)
6. Ensembles from the information theoretic perspective (*Chapter6.pdf*)
7. Fluctuations and the thermodynamic limit
8. Statistical mechanics of simple systems
9. Statistical mechanics of lattice models and introduction to models of solutions
    - Classical thermodynamic analog of solutions and mixtures (*Chapter2.pdf*)
10. A brief overview of statistical mechanics of liquids and soft-matter
11. Time permitting, we will cover some advanced topics
    - Non-equilibrium work relation and the statistical nature of the second law
    - Fluctuation dissipation theorem

Required and Suggested texts

Required texts:

1. Robert H. Swendsen, *An introduction to statistical mechanics and thermodynamics* — Cost is around \$75 (new) or $\approx$ \$50 (used)
    - This is labelled as an undergraduate text for a two semester course, but it is also very well suited for a graduate course and self-study
    - The positive reviews on Amazon correctly note that the concepts are well developed. Regarding the negative reviews, we will figure out the errors in the text, if any, as we go along.

2. Hill, *An introduction to statistical thermodynamics* (Dover edition; cost is about $ 18 (new) or $\approx$ $12 (old))

    - *This book should be part of the collection of any student who plans to work in statistical mechanics.* While I have moved away from Hill's development of the foundational concepts in statistical mechanics, the applications (and allied concepts) he develops cover a wide range that continue to be of significant interest in chemical and biomolecular sciences.

3. Course notes will be posted after each unit that we cover. These notes will refer to texts not listed here. It is left to the graduate student to see if he/she wants to also look into those texts.

Suggested reading:

1. Callen, *Thermodynamics and an Introduction to Thermostatistics* (1985)

    - **This is a classic and should be read by anyone intending to specialize in thermodynamics and statistical mechanics.** Callen was Swendsen's advisor, and Swendsen's text is greatly influenced by Callen's approach. Together with Welton, he is also famous for proving the fluctuation-dissipation theorem, a cornerstone result in equilibrium and non-equilibrium statistical mechanics.

2. Pathria and Beale, *Statistical Mechanics* (2011)

    - This is an excellent text. Has an excellent discussion of phase transitions, fluctuations, and introduction to computer simulations. There is also a chapter on the thermodynamics of the early universe!

3. Reif, *Fundamentals of Statistical and Thermal Physics* (Berkeley Physic Course)

    - This is a gem of a book that has been reissued recently. We used this during my undergraduate studies (as part of our physics curriculum). Has an excellent discussion of basics and some advanced topics.

4. Dill *Molecular driving forces — Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience (2nd edition)*

    - Dill derives useful insights from simple lattice models, but the simplifications are not without pitfalls. Useful to see possible applications.

Course Organization

The course will be structured around non-pledged assignments, a midterm, and a final that will be a combination of written and oral examinations.

- **Weekly non-pledged assignments**: For the non-pledged assignments you are free to discuss with your classmates, the TA, or instructor, and refer to other sources.
- **Periodic assessment**: We will have regular quizzes that I expect to deliver within Canvas. You are bound by the honor code for these assessments.

- **Midterm exam**: You are bound by the honor code.
- **Final exams**: You are bound by the honor code.

Honor code Policy

For non-pledged assignments, students are encouraged to discuss with each other, the teaching assistant, and the instructor. For all other work, you are prohibited from discussing the work with each other or use resources outside those that are explicitly allowed.

ADA Statement

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the **first two weeks of class**. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Allen Center.

Celebrating learning

Grade	%
Non-pledged Assignments	30
Periodic assessment (pledged)	10
Midterm (pledged)	20
Final (pledged)	40 (oral 20 + written 20)

Late assignments will incur penalties. Within 6 hours of the deadline we will deduct 5%. For anything more, we will deduct 10% for the first day and 10% each subsequent day.

Provisionally, we intend to follow grading based on the absolute scale noted below:

Grade	%	Grade	%
A+	≥ 99	C+	$63.0 - 68.9$
A	$93.0 - 98.9$	C	$57.0 - 62.9$
A-	$87.0 - 92.9$	F	< 57
B+	$81.0 - 86.9$		
B	$75.0 - 80.9$		
B-	$69.0 - 74.9$		

Only if the conditions demand, will we revisit the scale. Any changes will be adopted only after being voted on by the entire class.